

Semiclassical Quantisation Using Diffractive Orbits

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(February 5, 2008)

Abstract

Diffraction, in the context of semiclassical mechanics, describes the manner in which quantum mechanics smooths over discontinuities in the classical mechanics. An important example is a billiard with sharp corners; its semiclassical quantisation requires the inclusion of diffractive periodic orbits in addition to classical periodic orbits. In this paper we construct the corresponding zeta function and apply it to a scattering problem which has only diffractive periodic orbits. We find that the resonances are accurately given by the zeros of the diffractive zeta function.

PACS numbers: 0.320.+i, 03.65.Sq

Periodic orbit theory [1] encapsulates the duality between local, classical information such as the periods, actions and stabilities of periodic orbits and global quantum information such as the density of states. Because of its reliance on classical mechanics, the theory encounters difficulties whenever the classical mechanics is singular. Examples of singularities include three-body collisions as in the Helium atom [2]; grazing conditions where some trajectories hit a smooth billiard surface while very close, parallel trajectories do not [3]; bouncing from a wedge where trajectories on one side of the vertex are reflected differently from those on the other side [4–6]; and, scattering from a point scatterer [7,8] or a magnetic flux line [8] for which trajectories can not be continued through the discontinuities. In all of these examples, quantum mechanics smooths over the discontinuities through diffraction.

In what follows, we study the third example - that of wedges. If one is interested in finding the trace of the Green function $g(E) = \text{Tr}G(E)$ (and hence the density of states through $\rho(E) = -\text{Im}g(E)/\pi$) of such a system, one must include the effect of not just classical periodic orbits but also so-called diffractive orbits [4–6]. These are paths which go directly into at least one vertex. Such paths obey classical mechanics everywhere but at the vertex. There one allows the path to enter and leave the vertex at any angle [9] by assigning it an amplitude obtained by comparison with the exact solution of the quantum scattering problem [10].

This leads to the result that the contribution to the Green function of a diffractive path from point \mathbf{q}_A to \mathbf{q}_B via the vertex \mathbf{q}_V is approximately [4,9]

$$G_d(\mathbf{q}_B, \mathbf{q}_A, k) \approx G_f(\mathbf{q}_B, \mathbf{q}_V, k) d(\theta, \theta') G_f(\mathbf{q}_V, \mathbf{q}_A, k). \quad (1)$$

Henceforth we assume a billiard system in two dimensions so that $G_f(\mathbf{q}_2, \mathbf{q}_1, k) = -iH_0^{(+)}(k|\mathbf{q}_2 - \mathbf{q}_1|)/4$. The diffraction constant is [4,6]

$$d(\theta, \theta') = -\frac{4 \sin(\pi/\nu)}{\nu} \frac{\sin(\theta/\nu)}{[\cos(\pi/\nu) - \cos((\theta + \theta')/\nu)]} \frac{\sin(\theta'/\nu)}{[\cos(\pi/\nu) - \cos((\theta - \theta')/\nu)]}. \quad (2)$$

The angles θ and θ' are the incoming and outgoing angles relative to the same face of the wedge, although the choice of face is arbitrary. The wedge is parameterised by $\nu = \alpha/\pi$

where α is the opening angle of the wedge. We have assumed Dirichlet boundary conditions on all surfaces. Note that $d(\theta, \theta') = 0$ when $\alpha = \pi/n$. For these special angles, we can continue any trajectory through the vertex by flipping the wedge n times to cover the plane [6]. In that event, the contribution to the Green function is not diffractive but geometric with a phase factor of $(-1)^n$ due to the n specular reflections all trajectories experience in the wedge. Eq. (1) is approximate and valid for the points A and B far from the vertex. The approximation breaks down when $\theta \pm \theta' = \pi$, a condition which corresponds to the outgoing angle being directly on the border between a shadowed and an illuminated region as defined by the incoming angle. We return to this problem later.

As with geometric orbits, the trace of G is a sum over periodic orbits. A stationary phase evaluation yields the contribution of a periodic diffractive orbit labelled γ as [5,6]

$$g_\gamma(k) = -\frac{il_\gamma}{2k} \left\{ \prod_{j=1}^{\mu_\gamma} \frac{d_{\gamma,j}}{\sqrt{8\pi k l_{\gamma,j}}} \right\} \exp \{i(kL_\gamma + n_\gamma\pi - 3\mu_\gamma\pi/4)\}. \quad (3)$$

The diffractive orbit has μ_γ intersections with a vertex (diffractions) each with a corresponding diffraction constant $d_{\gamma,j}$ and n_γ reflections off straight hard walls. The total length of the orbit $L_\gamma = \sum l_{\gamma,j}$ is the sum of the lengths of the diffractive legs along the orbit and l_γ is the length of the corresponding primitive orbit. If the orbit γ is itself primitive then $L_\gamma = l_\gamma$. If γ is the m 'th repeat of some shorter orbit β , then $l_\gamma = l_\beta$, $L_\gamma = ml_\beta$, $n_\gamma = mp_\beta$ and $\mu_\gamma = m\sigma_\beta$. We then write

$$g_\gamma = g_{\beta,m} = -\frac{il_\beta}{2k} t_\beta^m \quad (4)$$

where

$$t_\beta = \left\{ \prod_{j=1}^{\sigma_\beta} \frac{d_{\beta,j}}{\sqrt{8\pi k l_{\beta,j}}} \right\} \exp \{i(kl_\beta + p_\beta\pi - 3\sigma_\beta\pi/4)\}. \quad (5)$$

This follows because the contributions from the various diffractive legs in Eq. (3) are multiplicative so that $g_{\beta,m}$ can be factorised. This is not true for geometric (nondiffractive) periodic orbits.

As with geometric orbits [11], we can organise the sum over diffractive orbits as a sum over the primitive diffractive orbits and a sum over the repetitions

$$g_d(k) = \sum_{\beta} \sum_{m=1}^{\infty} g_{\beta,m} = -\frac{i}{2k} \sum_{\beta} l_{\beta} \frac{t_{\beta}}{1-t_{\beta}}. \quad (6)$$

We cast this as a logarithmic derivative by noting that $\frac{dt_{\beta}}{dk} = il_{\beta}t_{\beta} - \sigma_{\beta}t_{\beta}/2k$ and recognising that the first term dominates in the semiclassical limit. It follows that

$$g_d(k) \approx \frac{1}{2k} \frac{d}{dk} \left\{ \ln \prod_{\beta} (1 - t_{\beta}) \right\}. \quad (7)$$

In addition to the diffractive orbits, one must also sum over the geometric (nondiffractive) periodic orbits so that in the logarithmic derivative we should also multiply by the contributions from the geometric orbits [3]. In what follows, we assume that all periodic orbits are diffractive so that the poles of $g(k)$ are the zeros of the zeta function [12–14]

$$\zeta^{-1}(k) = \prod_{\beta} (1 - t_{\beta}). \quad (8)$$

For geometric orbits, this is evaluated using a cycle expansion [13,14]. Here the weights t_{β} are multiplicative so the zeta function is a finite polynomial conveniently represented as the determinant of a Markov graph [15].

It is instructive to consider a system which can be quantised solely in terms of periodic diffractive orbits, such as the geometry of Fig. 1. The classical mechanics consists of free motion followed by specular reflections off the sides of the wedges. The two vertices are sources of diffraction. The choice $\gamma_1 = \gamma_2$ has been used to study microwave waveguides and conduction in mesoscopic devices and is known to have at least one bound state [16,17]. Unfortunately, in this case $\theta + \theta' = \pi$ for the periodic orbits labelled B and B' in Fig. 1b; Eq. (2) then diverges and the diffractive picture breaks down, as mentioned above. Instead, we consider $\gamma_1 > \gamma_2$. This is an open system with no bound states, only scattering resonances. As these are poles of $g(k)$ and hence zeros of $\zeta^{-1}(k)$ we can test the effectiveness of the theory in predicting them.

In what follows, we consider the case $\gamma_2 = 0$ for which the exact results are simple to obtain. (All the analytical results, however, are valid for $\gamma_2 \neq 0$). We define four cases: i) $\gamma_1 = \pi/2$; ii) $\gamma_1 > \pi/2$; iii) $\gamma_1 = \pi/2n$ ($n > 2$); and iv) all other values of γ_1 . Cases i) and

iii) differ from ii) and iv) respectively in that γ_1 corresponds to a special geometric angle and the lower vertex is not a source of diffraction. The reflection symmetry of the problem implies that all resonances are either even or odd. As a result, the zeta function factorises as $\zeta^{-1} = \zeta_+^{-1}\zeta_-^{-1}$ and we determine ζ_+^{-1} and ζ_-^{-1} separately.

For cases i) and ii) there is only one periodic diffractive orbit which is labelled A in Fig. 1a. In the first case there is only one diffraction point while in the second case there are two. The weight of the periodic orbit in the two cases is found from Eq. (5) as $t_A = d_{AA} \exp\{i(2kL + \pi/4)\}/\sqrt{16\pi kL}$ and $t_A = d_{AA}d'_{AA} \exp\{i(2kL + \pi/2)\}/8\pi kL$ respectively. The diffraction constants d_{AA} and d'_{AA} refer to diffraction from the top and bottom vertices respectively and can be found from Eq. (2). The resonances are determined by $t_A = 1$ which yields (to leading order) [5]

$$\begin{aligned} i) \quad kL &\approx n\pi - \pi/8 - \frac{i}{2} \ln \left(\frac{\sqrt{16\pi(n\pi - \pi/8)}}{d_{AA}} \right) \\ ii) \quad kL &\approx n\pi - \pi/4 - \frac{i}{2} \ln \left(\frac{8\pi(n\pi - \pi/4)}{d_{AA}d'_{AA}} \right) \end{aligned} \quad (9)$$

where n is a positive integer. Because the sole periodic orbit is on the symmetry axis, all of the resonances are predicted to be of even parity [18]. Unlike scattering systems quantised with geometric orbits [3,5,13,19], here there are no subleading resonances, a fact also observed in Refs. [5,7]. This is a result of the multiplicativity of the Green function (1).

For comparison, the exact resonances are found as follows. Defining polar coordinates with respect to the lower vertex, we expand the (unnormalisable) resonance wave function as

$$\begin{aligned} \psi(r, \theta) &= \sum_{n=1}^{\infty} a_n \sin(\alpha_n \theta) J_{\alpha_n}(kr) \quad r \leq L \\ &= \sum_{n=1}^{\infty} b_n \sin(\beta_n \theta) H_{\beta_n}^{(+)}(kr) \quad r \geq L, \end{aligned} \quad (10)$$

where $\alpha_n = (2n + 1)\pi/2\gamma_1$ and $\beta_n = n\pi/\gamma_1$. This satisfies all the boundary conditions and we have restricted the discussion to even resonances. Demanding that the wavefunction and its normal derivative be continuous along the arc $r = L$ gives the quantisation condition $\det M = 0$ where

$$M_{nm} = (-1)^{n+m} \frac{2}{\pi} \frac{n}{n^2 - (m - 1/2)^2} W_{nm}(kL) \quad (11)$$

and $W_{nm}(z)$ is the Wronskian of $J_{\alpha_m}(z)$ and $H_{\beta_n}^{(+)}(z)$. This relatively simple solution is a result of taking $\gamma_2 = 0$.

The results for both the exact resonances and their semiclassical approximations are shown in Fig. 2a for $\gamma_1 = \pi/2$ and $\gamma_1 = \pi - 0.5$. The weight t_A is greater by $O(\sqrt{kL})$ in the first case so that the resonances are not as unstable (i.e. not as far down in the complex k plane.) Although the agreement is very good, the theory is not very rich since it is based on just one periodic orbit. Of greater interest is a situation in which there are more diffractive orbits. As γ_1 is decreased, a pair of diffractive orbits is born each time γ_1 passes through a special angle $\pi/2n$. In particular, for $\pi/4 \leq \gamma_1 < \pi/2$ there are three fundamental periodic orbits [14], as sketched in Fig. 1b, together with an infinite hierarchy of longer orbits labelled by their itineraries among the points A , B and B' . For the special case $\gamma_1 = \pi/4$, the lower vertex is not diffractive but rather induces two specular reflections.

The weight of any orbit in which a letter is repeated can be expressed as the product of shorter weights (eg. $t_{ABB'B} = t_{AB}t_{B'B}$.) This means that the system can be written as a finite transfer matrix and the zeta function is the determinant of the corresponding Markov graph [20]. Due to the parity symmetry of the problem, we can consider just the right half of Fig. 1b as the fundamental domain. Fig. 3 is the Markov graph of the system and shows all the ways of connecting points A and B . For example, the line marked as 1 denotes starting at point B , going to the upper vertex and diffracting back. Symbols with a bar over them correspond to ending on the left half of the figure and then reflecting back onto the fundamental domain. For example, $\bar{2}$ denotes starting at B diffracting via the upper vertex to B' and then reflecting back onto B . Barred symbols contribute with a relative positive (negative) sign for the even (odd) resonances [18]. Symbol 5 is a so-called boundary orbit which lies on the border of the fundamental domain and contributes only to the even resonances. Each symbol carries its own weight and these combine to give the weights of the periodic orbits. To find an expression for the zeta function, we enumerate all

non-intersecting closed loops and non-intersecting products of closed loops to obtain [20]

$$\zeta_{\pm}^{-1} = 1 - t_1 \mp t_2 - t_3(t_4 \pm t_{\bar{4}}) - \frac{1 \pm 1}{2}(t_5 - t_5 t_1 \mp t_5 t_2). \quad (12)$$

Since by symmetry $t_4 = t_{\bar{4}}$, we have

$$\begin{aligned} \zeta_+^{-1} &= 1 - t_1 - t_2 - t_5 - 2t_3 t_4 + t_5(t_1 + t_2) \\ \zeta_-^{-1} &= 1 - (t_1 - t_2). \end{aligned} \quad (13)$$

We must still define the weights which appear in these formulas. Each symbol is composed of two segments leading from the corresponding nodes to the vertex connected by one diffraction at the vertex. We make use of this fact by separately defining quantities which contain the information about the segments and about the diffractions. The segment information is contained in u_A and u_B which are given by $u_A^2 = d'_{AA} \exp\{i(2kL - 3\pi/4)\}/8\pi kL$ for $\gamma_1 > \pi/4$ or $u_A^2 = \exp\{i2kL\}/\sqrt{16\pi kL}$ for $\gamma_1 = \pi/4$, and $u_B^2 = \exp\{i(2kH + \pi)\}/\sqrt{16\pi kH}$. These are simply the square roots of the weights of the fundamental periodic orbits shown in Fig. 1b but without the phase and diffraction constant from the vertex. That information we quantify by defining the phase factor $s = \exp\{-i3\pi/4\}$ and four diffraction constants. There is a constant to diffract from A back to itself which for $\gamma_2 = 0$ is $d_{AA} = 2$. With similar notation we find $d_{AB} = 2 \csc(\gamma_1/2 + \pi/4)$ and $d_{BB} = d_{BB'} = 1 + \csc \gamma_1$. (Note that by symmetry $d_{ij} = d_{ji}$.) The equality of d_{BB} and $d_{BB'}$ is an artifact of choosing $\gamma_2 = 0$ and is not a general result. We then have $t_1 = s d_{BB} u_B^2$, $t_2 = s d_{BB'} u_B^2$, $t_3 = t_4 = t_{\bar{4}} = s d_{AB} u_A u_B$ and $t_5 = s d_{AA} u_A^2$.

We stress that the only difference between cases iii) and iv) is the form of u_A and that the functional form (12) applies to both. However, as we will see, the numerical results are quite different. Due to the equality of d_{BB} and $d_{BB'}$, the weights t_1 and t_2 are equal so there are no odd resonances. This can also be seen from the fact that $J_\nu(z)$ and $H_\nu^{(+)}(z)$ are independent functions so there can be no odd resonances which satisfy all the boundary conditions and match smoothly at $r = L$.

We show the results for the even resonances for the cases $\gamma_1 = \pi/3$ and $\gamma_1 = \pi/4$ in Figs. 2b and 2c respectively. In the first case there is a diffraction at the lower vertex so

that $u_A/u_B = O(1/\sqrt{kL})$. Therefore the dominant behaviour for ζ_+^{-1} is dictated by t_1 and t_2 and the other terms represent small corrections. This is apparent in the figure where the gross behaviour is similar to Fig. 2a but with a decreasing, oscillatory correction coming from u_A . In the second case u_A is of the same order as u_B so that t_1 , t_2 and t_5 are all of similar magnitude. Then the resonances have no obvious pattern but are scattered around the complex k plane because of strong interferences among the various terms in ζ_+^{-1} .

In both cases the semiclassical approximation is very accurate. In addition it gives us a better qualitative understanding of the spectrum than the exact numerical calculation based on Eq. (10). Although we can not yet study the case $\gamma_1 = \gamma_2$ in detail, we can begin to understand why none of its bound states are odd [17]. Recall that bound states correspond to real zeros of the zeta functions. However, the odd zeta function receives no contribution from the boundary orbit and also suffers from strong cancellation due to the relative negative sign between t_1 and t_2 , so only quite far from the real k axis are the magnitudes of the weights sufficiently large to allow for a zero. It is reasonable to suppose that this general condition continues to hold as $\gamma_1 \rightarrow \gamma_2$. However, a complete semiclassical analysis of this case requires an understanding of the behaviour of the Green function on the border between shadowed and illuminated regions.

Finally, we mention that the restriction to $\gamma_1 \geq \pi/4$ is not crucial. For smaller values of the angle, more diffractive orbits appear but the formalism above still applies and can be used to find the corresponding zeta function.

I thank Stephen Creagh, Predrag Cvitanović, Peter Dimon, Julie Lefebvre, Gregor Tanner, Gábor Vattay and Andreas Wirzba for useful discussions. This work was supported by the EU Human Capital and Mobility Programme.

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FIGURES

FIG. 1. a) A configuration with only one diffractive periodic orbit. b) A configuration with an infinity of diffractive periodic orbits labelled by their itineraries among A , B and B' .

FIG. 2. The resonances in the complex k plane. a) Results with only one diffractive periodic orbit. The upper set of points corresponds to $\gamma_1 = \pi/2$ and the lower set corresponds to $\gamma_1 = \pi - 0.5$. For each set, the exact resonances are denoted with crosses and the semiclassical approximations with diamonds. With the same convention, b) shows the results for $\gamma_1 = \pi/3$ and c) shows the results for $\gamma_1 = \pi/4$.

FIG. 3. The Markov graph used to compute the desymmetrised zeta functions.